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Effect of chiral interactions in frustrated magnetic chains

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The Heisenberg model with competing exchanges together with the chiral term is studied using series expansion about the dimer limit and by finite-size diagonalizations. The phase diagram is determined with ground-state orderings and the lowest excitation characteristics. We find that the chiral term induces a gapless line in frustrated spin-gapped phases. A critical chiral strength is also able to change the ground state from spiral to Néel quasi-long-range-order phase.

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The ground-state and the low-energy excitations of the quasi-one-dimensional quantum antiferromagnets have been extensively studied in the last decades.[1] The effect of a magnetic field on such systems is mostly described by the Pauli term, wherein the field couples with the z component of the total spin of the system. This term splits the finite magnetization spin levels and, for an antiferromagnet with a nonmagnetic ground state, a stronger field can even produce a high-spin state as the ground state. However, electrons have both the charge as well as the spin degrees of freedom. The quantum antiferromagnetic Heisenberg model is derived from the fermionic Hubbard model in a second-order perturbation theory, where the charge degrees of freedom are frozen (in the large Hubbard U limit).[2] With the magnetic field term in the Hubbard model, the perturbation does not result in any interesting terms for a bipartite lattice. However, for a nonbipartite lattice, as has been shown, the magnetic field can couple with the spin and produce a new term in the perturbation apart from the usual Heisenberg-type spin models.[3] This new term is of the form $S_i \cdot S_j \times S_k$, where S_i is the spin at site i, and its effect has not been explored thoroughly for frustrated magnetic chains.

In general, in an antiferromagnet, the ground state is a singlet. Since the Pauli term does not couple to the nonmagnetic state, it is not clearly understood whether the singlet state would couple to the chiral term and, in that case, whether the Pauli term would compete with the chiral term in producing a magnetic ground state. Such a situation is quite unlikely to occur, since the chiral term arises in the third-order perturbation theory, the magnitude of which is proportional to t^3/U^2, where t is the hopping strength.[4] Despite this, it has been speculated that in certain cases the chiral term may have a larger effect on the ground state than the Pauli coupling, thereby drastically affecting the ground-state properties.[3] One example is the case where the ground state is doubly degenerate in zero field with opposite chiralities. In that case, when an external magnetic field is applied, the chiral degeneracy is broken by the chiral term. The Pauli interaction term, however, has no effect on the ground state for fields smaller than the lowest spin gap.[4]

On the other hand, the low-dimensional materials with competing exchange interactions have generated a huge interest because of their unique low-energy characteristics. The Heisenberg model with nearest- and next-nearest-neighbor interactions produce a rich phase diagram with gapless and gapped phases as a function of the frustration. The next-nearest-neighbor term, which causes frustration, spontaneously dimerizes the system after a certain critical value, and the phase diagram has been quite well established.[5]

The Heisenberg model with competing exchanges, together with this chiral term, is integrable for certain parameters. It has been recently found that a finite chiral field term can lift the degeneracy associated with the Majumdar-Ghosh point with a nonzero chiral expectation value.[6] For a unique ground state, the Hamiltonian remains parity and time symmetric, leading to a vanishing chirality in the ground state. On the other hand, a two-dimensional spin-1/2 Heisenberg model on a square lattice, frustrated with a sufficiently strong antiferromagnetic next-nearest-neighbor interaction, has been proposed to have a chiral ground state.[7] Subsequent studies of this two-dimensional model have found an enhancement of the chiral order parameter, although comparison with other possible states suggests that the chiral spin state is quite unstable.[8] Different lattices, in particular the triangular and Kagome systems, have also been studied, however, no firm evidence of chiral spin state has been found so far.[6]

Given that the strength of the chiral term is quite small and that it is quite impossible to stabilize the singlet over the magnetic state when a magnetic field is applied, it would be quite interesting to ask whether the chiral term can give rise to changes in the nature of the ground-state and low-energy excitations of the low-dimensional frustrated systems. To understand its effect in reduced dimension, we analyze a quasi-one-dimensional frustrated system, the exchange Hamiltonian for which can be written as (see Fig. 1)

$$H = J_1 \sum_i S_i \cdot S_{i+1} + J_2 \sum_i S_i \cdot S_{i+2}, \tag{1}$$

where J_1 and J_2 are the nearest- and second-neighbor exchange interactions, respectively. We define $J = J_2/J_1$, where

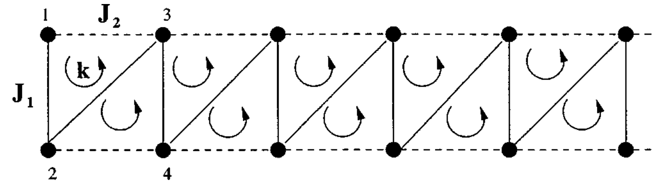

FIG. 1. Picture of the lattice considered in the Hamiltonian. The directions of the chiral interaction are shown as curved arrows.

J_1 is fixed at 1. For $J=0$, the model is exactly soluble by the Bethe *ansatz* model.[9,10] For $J \neq 0$, the ground-state phase diagram has been extensively studied both analytically and numerically.[11–14] These studies have revealed that when $J \leqslant J_c$, the system is in a gapless spin-fluid phase in which the antiferromagnetic spin correlations decay algebraically. In contrast, for $J \geqslant J_c$, the system is in a completely different phase, characterized by a finite excitation gap and exponential decay of the spin correlation functions. The value of J_c has been accurately computed to be 0.2411 ± 0.0001.[5,15] Interestingly, this model can be solved exactly for $J=0.5$. The ground state is doubly degenerate with exact dimeric forms.[16]

To force the system into a chiral spin state, we add the following term:

$$H' = K\sum_i \left[S_{2i-1} \cdot (S_{2i} \times S_{2i+1}) + S_{2i} \cdot (S_{2i+2} \times S_{2i+1})\right], \tag{2}$$

where K is the chiral interaction strength.

In the following, we present a systematic study of the various regions of the phase diagram in the J–K phase plane using a dimer expansion[17,18] and finite-size diagonalization methods. In order to obtain an idea of the energy-level structure, we have carried out finite-size diagonalization for system sizes, $N=8-20$ spins with periodic boundary conditions. The ground state is found to be a singlet all over the phase diagram.

To understand the low-energy characteristics of the system in the J–K phase plane, we have kept the J value fixed and have varied the K value from 0 to 1. This has been done for various values of J. We calculate the singlet-singlet gap, Δ_{ss}, and singlet-triplet gap, Δ_{st}, for all the system sizes in the J–K phase space. Δ_{st} gives us an indication that as a function of K, the system goes through a gapless point for every value of J above J_c. To determine these gapless points, we plot both the Δ_{ss} and Δ_{st} values for various values of K, for every J. Figure 2 shows the nature of these two gaps in the gapless ($J=0.1$) and in gapped ($J=0.6$) phases for a $N=20$ sites ring. For J below J_c, the spin gap, as well as the singlet-singlet gap, increase as a function of K, indicating that the chiral term does not couple strongly with any of the low-energy states. In fact, for large $K(K \to 1)$, we find that the chiral term couples with the lowest triplet state little stronger than the ground state and in that limit the spin gap is quite large. However, for $J > J_c$, there is a finite spin gap to start with for $K=0$, and interestingly, the spin gap decreases with the increase in K value for small K values. Nevertheless, above a certain critical K for every $J > J_c$, it increases again. Furthermore, we find that the chiral term couples quite strongly to the lowest triplet state at small K values, above which it couples quite equally to both the ground state and magnetic state.

We have carried out computations of these gap parameters for various values of J for a number of system sizes. The special point of $J=0.5$ is worth mentioning. At $K=0$, the ground state is the exact dimer states. But as we introduce K, this exact dimer degeneracy is lifted, since the correlation between the dimers becomes finite. The ground state in that case cannot be expressed in product dimer forms, although there remains a finite spin gap all over the K line except at around $K=0.4$, where it is nondegenerate with gapless excitations.

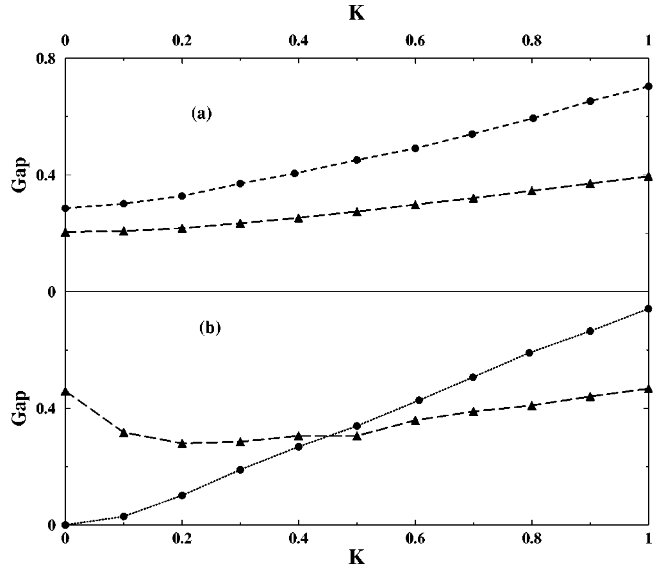

FIG. 2. Lowest singlet-singlet (Δ_{ss}, circles) and singlet-triplet (Δ_{st}, triangles) gaps for (a) $J=0.1$ and (b) $J=0.6$ from exact diagonalization studies of a 20 sites ring.

As discussed above, for every value of $J > J_c$, there exists a critical K point, $K_c(N)$, corresponding to the crossing of the Δ_{ss} and Δ_{st} curves, for a given system size, N. To obtain these critical K points in the thermodynamic limit, we adopt the method suggested by Okamoto and Nomura, where one plots the finite-size critical points as a function of $1/N^2$. The least-squares fitting of the equation $K_c(N)=K_c+\text{const}/N^2$ then gives the value of the critical points (K_c) in the thermodynamic limit.[15]

Additionally, we have also carried out series expansion calculations to obtain ground-state energy, structure factor, and the singlet-triplet excitation spectrum for input parameters J and K. This method has been previously described in several articles,[17–19] and will not be repeated here. We would just like to add that since our Hamiltonian is a complex hermitian, we had to be diligent in computing its properties.

In the limit that the exchange coupling along the rungs J_1 and J_2 are much larger than the couplings K, the Hamiltonian can be written as

$$H = H_0 + \lambda V, \tag{3}$$

where

$$H_0 = \sum_i S_{2i-1} \cdot S_{2i},$$

$$V = \sum_i S_{2i} \cdot S_{2i+1} + J\sum_i S_i \cdot S_{i+2} + K\sum_i \left[S_{2i-1} \cdot (S_{2i} \times S_{2i+1}) + S_{2i} \cdot (S_{2i+2} \times S_{2i+1})\right]. \tag{4}$$

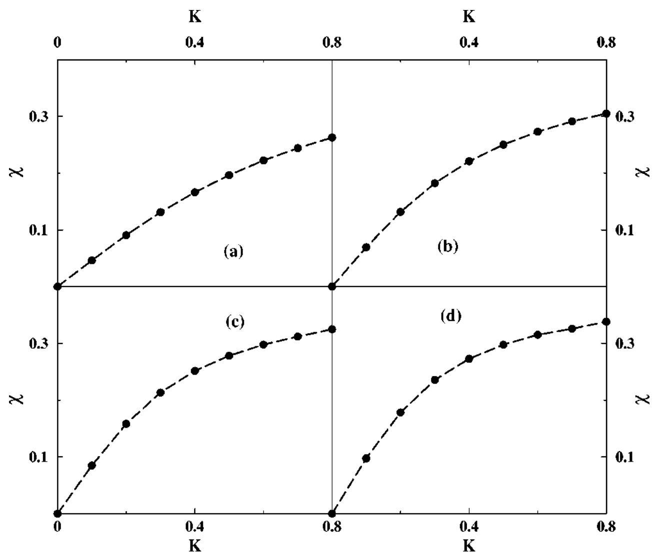

FIG. 3. Order parameter as a function of K from series expansion, for J values (a) 0.1, (b) 0.3, (c) 0.4, and (d) 0.5.

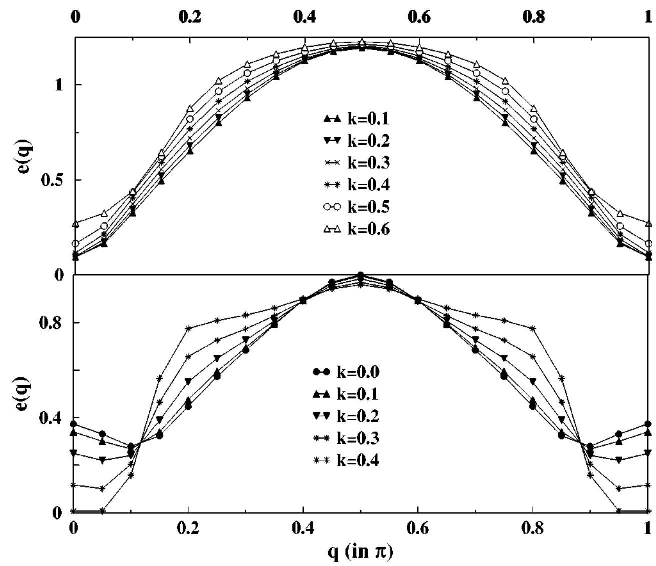

FIG. 4. The triplet dispersion curve, $e(q)$ vs q, for various values of K at (a) $J=0.3$ and (b) $J=0.5$.

We can obtain an expansion in λ by treating the operator H_0 as the unperturbed Hamiltonian, and the operator V as the perturbation. This dimer expansions have been carried out up to the order λ^{11} for the ground state and to the λ^{10} order for the excited states, with the graph size of 11 and 10 dimers, respectively, for every parameter values. Our expansion code with $K=0$ reproduces the results obtained for the $J_1-J_2-\delta$ model.[20]

To characterize a phase transition, an order parameter has to be introduced. We define the chiral order parameter as

$$\chi = 1/N\sum_{i=1}^{N}\left[S_{2i-1}\cdot(S_{2i}\times S_{2i+1}) + S_{2i}\cdot(S_{2i+2}\times S_{2i+1})\right]. \tag{5}$$

In Fig. 3, we plot the order parameters as a function of the chiral interaction strength for four different J values. As can be seen, for J below J_c, the order parameter increases with K with the same slope without any features. However, for J above J_c, it shows the change in the slope around a particular K point, which exactly supports the finite-size diagonalization results. More specifically, for $J=0.3$, the slope of the order parameter changes around $K=0.2$. For $J=0.4$ and 0.5, this occurs around $K=0.3$ and 0.4, respectively. At the special point, at $J=0.5$, along the K line, the results are quite interesting. At $K=0.0$, the values of all the correction terms of the energy are zero as expected and the dimer energy is $-3J/4$. However, the energy correction is finite as we switch on the K, indicating that the chiral field lifts the ground-state dimer degeneracy.

To understand the excitation characteristics in the K line for various values of J, we compute the excitation energy using series expansion. The spin gap is generally defined as the minimum energy point in the $e(q)$ vs q plot, where $e(q)$ is energy gap to the triplet state at a wave vector q.[21] For $J<J_c$, we find that increase in K increases the singlet-triplet gap, while for J above J_c, the gap reduces with K up to a certain K, where the gap vanishes. The $e(q)$ vs q is shown in Fig. 4, for $J=0.3$ and 0.5, for a number of K values. For $J=0.3$, the gap is very small up to the critical $K=0.2$, above which it starts increasing. For $J=0.5$, this excitation is gapless at $K=0.4$, while there is a finite gap for other K values. It is interesting to note that all the $J=0.5$ $e(q)$ curves cross at two particular q values and they are symmetric about $q=\pi/2$. The q values at those points are, however, incommensurate ($q\approx 0.12\pi$ and 0.41π). Moreover, the $e(q)$ curve for $K=0$ also crosses at those q values, suggesting the possibility of a common exact eigenstate for the Majumdar-Ghosh model with and without the chiral term. Note that the minimum in $e(q)$ is always found at $q=0$ or π and it is symmetric around $q=\pi/2$.

Next, we calculate the magnetic structure factor to further understand the nature of the ground-state ordering in gapless and gapped phases. In the J line with $K=0$, the classical spin limit ($S\rightarrow\infty$) predicts a Néel ordering for $J<0.25$ and a coplanar or spiral order for J above 0.25. In other words, $S(q)$ has a peak at $q_{max}=\pi$ for $J<0.25$ and at $q_{max}=\cos^{-1}(1/4J)$ for $J>0.25$. However, the quantum model has no long-range order (LRO), rather, it has a quasi-LRO of the order of the system size for the spin-1/2 case. For $S=1/2$, the Néel quasi-LRO exists up to $J\leqslant 0.5$, above which the systems goes into a spiral phase. The spiral phase in this case is characterized by the peak in the $S(q)$ at some q_{max} value between π and $\pi/2$.

At $K=0$, the series expansion $S(q)$ reproduces the known results. For $J\leqslant 0.5$, the $S(q)$ peaks at $q_{max}=\pi$, while it is at $q_{max}<\pi$ for $J>0.5$. With the introduction of K, the q_{max} value remains the same ($q_{max}=\pi$) for $J\leqslant 0.5$, for all K values. However, above $J=0.5$, to start with, for $K=0$, the q_{max} is less than π, and after introduction of K, the $S(q)$ remains peaked at the incommensurate values up to the K value where the excitation gap vanishes. Interestingly, the chiral term above a certain critical strength restores back the Néel quasi-LRO phase ($q_{max}=\pi$) from the incommensurate phase.

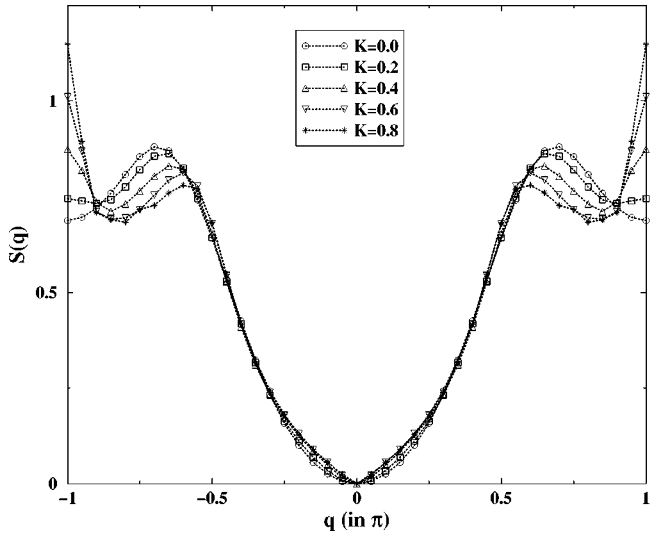

FIG. 5. Structure factor, $S(q)$ vs q for various values of K at J $=0.6$.

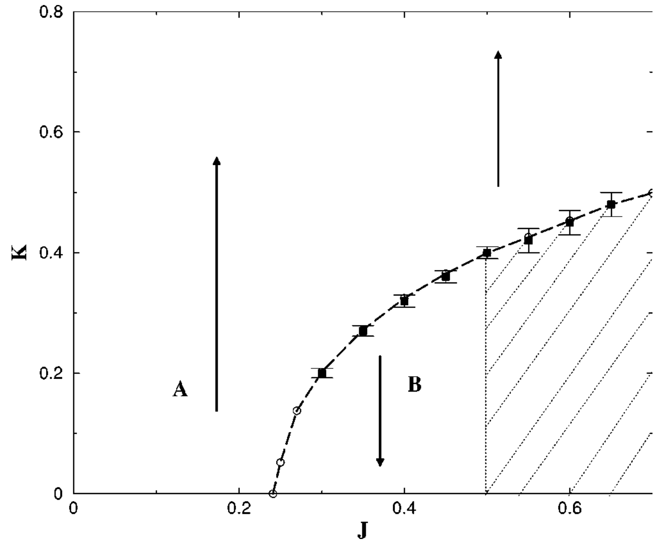

FIG. 6. Phase diagram in the $J-K$ phase plane. While A and B have the Néel quasi-long-range order, the shaded region has spiral order. The dashed line correspond to the gapless line, with open circles from finite-size scaling of the finite-size diagonalizations data and the filled squares with error bars from series expansion. The arrows indicate the behavior of the spin gap; the gap increases in the arrow directions.

In Fig. 5, we plot the $S(q)$ as a function of q at $J=0.6$, for a number of K values. As can be seen, the q_{max} value is incommensurate up to $K=0.4$, above which the q_{max} restores back to π.

Finally, we present the phase diagram of the above model in the $J-K$ phase plane in Fig. 6. Putting together all the above results for the finite sized systems with scaling and the series expansion, it is clear that there exist a gapless line in $J-K$ plane above $J>J_c$. All over the phase diagram, the system is in a Néel quasi-LRO phase except in the shaded region, where it is in spiral phase. While the gap increases with the increase in K values in phase A, in the case of phase B, the gap reduces with an increase in chiral strength up to the critical chiral values, above which it increases again with the increase in K. For $K=0$, as J increases above J_c, the spin gap increases, however, up to a certain J, above which it again decreases. The full phase diagram is shown in Fig. 6. The arrows indicate the increase of the spin gap towards the direction of the arrow. Since $K=0$ has been well studied for even large J, we present results up to $J\sim 0.7$.

To conclude, we have shown that although the strength of the chiral interaction is quite small, it can give rise to exotic phases specifically when the system becomes spontaneously dimerized due to frustrations. It can even change the ground-state ordering. We also found an existence of a gapless line in the $J-K$ phase plane.

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